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Calculation of the Potential Distribution for a Three-Layer Spherical Volume Conductor

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Introduction

Electroencephalography (EEG) and magnetoencephalography (MEG) are non-invasive methods of studying the functional activity of the human brain with millisecond temporal resolution. Much of the work in EEG and MEG in the last few decades has been focused on estimating the properties of the internal sources of the fields from the external measurements, i.e. on solving the inverse problem of EEG and MEG. To handle this task one must first study the forward problem, i.e. how the fields arise from a known source. For practical purposes, one also has to choose appropriate models for the source and the head as a conductor. The most straightforward model for describing the surface evoked potential or the external evoked magnetic field is the single equivalent current dipole. In EEG models the volume conductor properties of the head are commonly modelled by three or four concentric spherical shells with different electrical conductivities representing the brain, the cerebrospinal fluid, the skull, and the scalp [1-2]. While more accurate geometric models have been applied, such asymmetric models are limited in accuracy by knowledge of boundaries and resistivities of various tissues. In this article we consider a three-layer spherical volume conductor model and calculate the dipole-induced potential by analytical methods. This calculation requires the symbolic solution of a system of linear equations which is not complicated but that would be a pain when done by pencil and paper [1-3]. We use Maple for setting up the system of model equations, solve it symbolically, and then generate numerical code to obtain a fast program for the evaluation of the potential. Finally, the dipole-envoked electric potential is plotted for realistic EEG model parameters.

The intention of this interdisciplinary application is to illustrate how Maple can be used as an integrated working environment for investigating mathematical models as they occur in brain research.

Mathematical Model

Suppose $||\mathbf{r}|| = a, b, c$ define three concentric spherical surfaces with $0 < a < b < c < \infty$. We consider a current dipole with moment $\mathbf{Q}$ inside of surface $||\mathbf{r}|| = a$, i.e. we assume $r_Q = ||\mathbf{r}_Q|| < a$ for the dipole position vector $\mathbf{r_Q}$. The potential distribution $U(\mathbf{r})$ created by this

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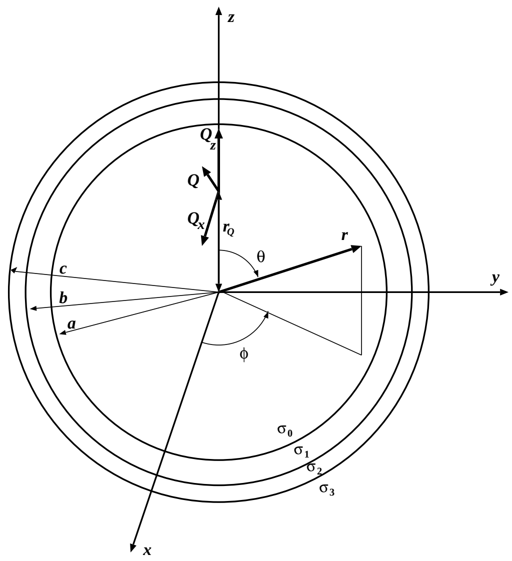

Figure 1: Three-layer spherical model of the head. The inner sphere represents the brain (a); the successive layers represent the skull (b) and the scalp (c). The dipole is on the z axis of the EEG coordinate system.

dipole is described by the Poission equation

$$\bigtriangledown^2 U(\mathbf{r}) = \bigtriangledown \bullet (\frac{\mathbf{Q}}{\sigma_0}\delta(\mathbf{r}-\mathbf{r}_Q)) = \frac{\mathbf{Q}}{\sigma_0} \bullet \bigtriangledown \delta(\mathbf{r}-\mathbf{r}_Q) \tag{1}$$

and the Laplace equation

$$\bigtriangledown^2 U(\mathbf{r}) = 0. \tag{2}$$

In Eq. (1) $\delta(\mathbf{r})$ is the Dirac delta funtion, $\bigtriangledown$ the gradient operator and σ_0 denotes the conductivity in the sphere $\|\mathbf{r}\| < a$. For solving these equations we consider the special case of a dipole located on the z axis and a moment vector $\mathbf{Q}$ which lies in the x-z plane (see Fig. 1). The multipole expansion for the electric potential in a volume conductor then yields the following formal solution [1]:

$$\begin{aligned} U(\mathbf{r}) &= U_0(\mathbf{r}) + U_a(\mathbf{r}), & 0 < \|\mathbf{r}\| < a, \\ &= U_b(\mathbf{r}), & a < \|\mathbf{r}\| < b, \\ &= U_c(\mathbf{r}), & b < \|\mathbf{r}\| < c, \\ &= U_d(\mathbf{r}), & c < \|\mathbf{r}\| < \infty, \end{aligned} \tag{3}$$

where

$$U_0(\mathbf{r}) = Ux_0(\mathbf{r}) + Uz_0(\mathbf{r}) \tag{4}$$

with

$$Ux_0(\mathbf{r}) = \sum_{l=1}^{\infty} \frac{Q_x}{4\pi\sigma_0} \frac{r_Q^{l-1}}{r^{l+1}} P_l^1(\cos(\theta))\cos(\phi), \tag{5}$$

and

$$Uz_0(\mathbf{r}) = \sum_{l=1}^{\infty} \frac{Q_z}{4\pi\sigma_0} \frac{l r_Q^{l-1}}{r^{l+1}} P_l(cos(\theta)), \tag{6}$$

is a special solution of the Poission equation inside of the sphere $||\mathbf{r}|| = a$ and

$$U_I(\mathbf{r}) = \sum_{l=1}^{\infty} A_l^I(r) f(\theta, \phi), \quad I = a, b, c, d, \tag{7}$$

with

$$f(\theta, \phi) = \begin{cases} P_l^1(\cos(\theta))\cos(\phi) & \text{for the } x \text{ component of } \mathbf{Q} \\ P_l^0(\cos(\theta)) & \text{for the } z \text{ component of } \mathbf{Q} \end{cases}$$

represent the series solutions of the Laplace equation in the various regions, assuming that the asymptotic behavior of the potential is given by $U(\mathbf{r}) \to 0$ as $||\mathbf{r}|| \to \infty$. Here, Q_x is the vertical component and Q_z the parallel component of the dipole moment $\mathbf{Q}$ with respect to the z axis, (r, θ, ϕ) denote the spherical coordinates of the position vector $\mathbf{r}$, and $P_l^n(u)$ stands for an associated Legendre polynomial. The coefficients $A_l^I(r), I = a, b, c, d$, are so far undetermined. If the dipole is not on the z axis, we first transform the coordinate system, and then calculate the potential with respect to a new coordinate system (x_new, y_new, z_new) in which the dipole is on the z_new axis. The coefficients will be determined by applying the boundary conditions that the potential and current flow must be continuous across the boundaries between regions of different conductivity. The electrical conductivities in the various regions are denoted by σ_0 for $||\mathbf{r}|| < a$, σ_1 for $a < ||\mathbf{r}|| < b$, σ_2 for $b < ||\mathbf{r}|| < c$, and σ_3 for $c < ||\mathbf{r}|| < \infty$.

Calculating the Potential distribution

In this section we give the analytical evaluation for the potential U produced by the x component Q_x of the dipole moment $\mathbf{Q}$. The calculation for the potential created by the z component Q_z is done in a similar way. Let a_P(l, n, u) denote a so far undefined Maple procedure for calculating the associated Legendre polynomials $P_l^n(u)$. Then, we have the following series solutions for the potential U in the various regions:

```
> Ux[0]:=Sum(Q[x]/(4*Pi*sigma[0])*rQ^(l-1)/r^(l+1)*a_P(l,1,cos(theta))*cos(phi),
> l=1..infinity);
```

$$Ux_0 := \sum_{l=1}^{\infty} \left(\frac{1}{4} \frac{Q_x \, rQ^{(l-1)} \, \mathrm{a\_P}(\, l, 1, \cos(\,\theta\,)\,) \cos(\,\phi\,)}{\pi \, \sigma_0 \, r^{(\,l+1\,)}} \right)$$

fulfills the Poisson equation. The potential which satisfies the Laplace equation inside of the spherical surface $||\mathbf{r}|| = a$ is given by

```
> Ux[a]:=Sum(A[l]*r^l*a_P(l,1,cos(theta))*cos(phi),l=1..infinity);
```

$$Ux_a := \sum_{l=1}^{\infty} A_l \, r^l \, \mathrm{a\_P}(\, l, 1, \cos(\,\theta\,)\,) \cos(\,\phi\,)$$

The coefficients $A_l, l \geq 1$, are so far unspecified. For the potential between the two spherical surfaces $||\mathbf{r}|| = a$ and $||\mathbf{r}|| = b$ we have

```
> Ux[b]:=Sum((B[l]/r^(l+1)+C[l]*r^l)*a_P(l,1,cos(theta))*cos(phi),l=1..infinity);
```

$$Ux_b := \sum_{l=1}^{\infty} \left(\frac{B_l}{r^{(l+1)}} + C_l\, r^l\right) \text{a\_P}(\, l, 1, \cos(\,\theta\,)\,) \cos(\,\phi\,)$$

Here, B_l and C_l are undetermined coefficients. For the potential between the two spherical surfaces $||\mathbf{r}|| = b$ and $||\mathbf{r}|| = c$ holds

```
> Ux[c]:=Sum((D[l]/r^(l+1)+E[l]*r^l)*a_P(l,1,cos(theta))*cos(phi),l=1..infinity);
```

$$Ux_c := \sum_{l=1}^{\infty} \left(\frac{D_l}{r^{(l+1)}} + E_l\, r^l\right) \text{a\_P}(\, l, 1, \cos(\,\theta\,)\,) \cos(\,\phi\,)$$

Again, D_l and E_l denote undetermined coefficients. The potential outside of the spherical surface $||\mathbf{r}|| = c$ is given by

```
> Ux[d] := Sum((F[l]/r^(l+1))*a_P(l,1,cos(theta))*cos(phi), l=1..infinity);
```

$$Ux_d := \sum_{l=1}^{\infty} \frac{F_l\, \text{a\_P}(\, l, 1, \cos(\,\theta\,)\,) \cos(\,\phi\,)}{r^{(\, l+1\,)}}$$

$F_l, l \geq 1$, are coefficients to be found. Inside of the surface $||\mathbf{r}|| = a$ the potential is $U_0 + U_a$, between the surfaces $||\mathbf{r}|| = a$ and $||\mathbf{r}|| = b$ the potential is U_b, and on the surface $||\mathbf{r}|| = a$ the potential should be continuous, i.e. $U_0 + U_a = U_b$ should hold, which in turn leads to the following equation for the terms of the corresponding infinite series representations:

```
> eqn_a := collect(op(1, Ux[0]) + op(1, Ux[a]) = op(1, Ux[b]),
> [a_P(l,1,cos(theta)),cos(phi)]);
```

$$eqn\_a := \left(\frac{1}{4}\,\frac{Q_x\; rQ^{(\,l-1\,)}}{\pi\,\sigma_0\, r^{(\,l+1\,)}} + A_l\, r^l\right) \cos(\,\phi\,)\, \text{a\_P}(\, l, 1, \cos(\,\theta\,)\,) = \left(\frac{B_l}{r^{(\,l+1\,)}} + C_l\, r^l\right) \text{a\_P}(\, l, 1, \cos(\,\theta\,)\,) \cos(\,\phi\,)$$

Simplifying and then substituting $r = a$ yields the first relation for the coefficients of the infinite series.

```
> eqn_a_0 := simplify(eqn_a/(a_P(l,1,cos(theta))*cos(phi)), power):
> eqn_a_1 := subs(r=a, eqn_a_0);
```

$$eqn\_a\_1 := \frac{1}{4}\,\frac{Q_x\; rQ^{(\,l-1\,)}\, a^{(\,-l-1\,)}}{\pi\,\sigma_0} + A_l\, a^l = B_l\, a^{(\,-l-1\,)} + C_l\, a^l$$

The current perpendicular to the surface $||\mathbf{r}|| = a$ should be continuous also, i.e. the potential should satisfy $\sigma_0 \frac{\mathrm{d}}{\mathrm{d}r}(U_0(r) + U_a(r))(a) = \sigma_1 \frac{\mathrm{d}}{\mathrm{d}r}(U_b(r))(a)$, which leads to the next relation for the coefficients.

```
> eqn_a_2 := simplify(subs(r=a, sigma[0]*diff(lhs(eqn_a_0), r)=
> sigma[1]*diff(rhs(eqn_a_0), r)), power);
```

$$eqn\_a\_2 := \sigma_0 \left(\frac{1}{4}\,\frac{Q_x\; rQ^{(\,l-1\,)}\, a^{(\,-l-2\,)}\,(\,-l-1\,)}{\pi\,\sigma_0} + A_l\, a^{(\,l-1\,)}\, l\right) = \sigma_1 \left(B_l\, a^{(\,-l-2\,)}\,(\,-l-1\,) + C_l\, a^{(\,l-1\,)}\, l\right)$$

On the surface $||\mathbf{r}|| = b$ the boundary condition for the potential, $U_b = U_c$, gives the equations

```
> eqn_b := op(1, Ux[b]) = op(1, Ux[c]);
```

$$eqn\_b := \left(\frac{B_l}{r^{(l+1)}} + C_l\, r^l\right) \text{a\_P}(\,l, 1, \cos(\,\theta\,)\,)\cos(\,\phi\,) = \left(\frac{D_l}{r^{(l+1)}} + E_l\, r^l\right) \text{a\_P}(\,l, 1, \cos(\,\theta\,)\,)\cos(\,\phi\,)$$

```
> eqn_b_0 := simplify(eqn_b/(a_P(l,1,cos(theta))*cos(phi))):
> eqn_b_1 := subs(r=b, eqn_b_0);
```

$$eqn\_b\_1 := B_l\, b^{(\,-l-1\,)} + C_l\, b^l = D_l\, b^{(\,-l-1\,)} + E_l\, b^l$$

The current perpendicular to the surface $\|\mathbf{r}\| = b$ satisfies the boundary condition $\sigma_1 \frac{\mathrm{d}}{\mathrm{d}r}(U_b(r))(b) = \sigma_2 \frac{\mathrm{d}}{\mathrm{d}r}(U_c(r))(b)$ which results in the following condition for the coefficients of the series solutions:

```
> eqn_b_2 := simplify(subs(r=b, sigma[1]*diff(lhs(eqn_b_0), r)=
> sigma[2]*diff(rhs(eqn_b_0), r)), power);
```

$$eqn\_b\_2 := \sigma_1 \left(B_l\, b^{(\,-l-2\,)}\,(\,-l-1\,) + C_l\, b^{(\,l-1\,)}\, l\right) = \sigma_2 \left(D_l\, b^{(\,-l-2\,)}\,(\,-l-1\,) + E_l\, b^{(\,l-1\,)}\, l\right)$$

The boundary conditon for the surface $\|\mathbf{r}\| = c$, given by $U_c = U_d$, implies the following conditional equations for the coefficients of the corresponding infinite series:

```
> eqn_c := op(1, Ux[c]) = op(1, Ux[d]);
```

$$eqn\_c := \left(\frac{D_l}{r^{(l+1)}} + E_l\, r^l\right) \text{a\_P}(\,l, 1, \cos(\,\theta\,)\,)\cos(\,\phi\,) = \frac{F_l\, \text{a\_P}(\,l, 1, \cos(\,\theta\,)\,)\cos(\,\phi\,)}{r^{(\,l+1\,)}}$$

```
> eqn_c_0 := simplify(eqn_c/(a_P(l,1,cos(theta))*cos(phi))):
> eqn_c_1 := subs(r=c, eqn_c_0);
```

$$eqn\_c\_1 := D_l\, c^{(\,-l-1\,)} + E_l\, c^l = F_l\, c^{(\,-l-1\,)}$$

Finally, the boundary condition for the current perpendicular to the surface $\|\mathbf{r}\| = c$, $\sigma_2 \frac{\mathrm{d}}{\mathrm{d}r}(U_c(r))(c) = \sigma_3 \frac{\mathrm{d}}{\mathrm{d}r}(U_d(r))(c)$, gives the last relation for the coefficients of the infinite series representations.

```
> eqn_c_2:=simplify(subs(r=c, sigma[2]*diff(lhs(eqn_c_0), r)=
> sigma[3]*diff(rhs(eqn_c_0), r)), power);
```

$$eqn\_c\_2 := \sigma_2 \left(D_l\, c^{(\,-l-2\,)}\,(\,-l-1\,) + E_l\, c^{(\,l-1\,)}\, l\right) = \sigma_3\, F_l\, c^{(\,-l-2\,)}\,(\,-l-1\,)$$

Now, solving the linear equations $eqn\_a\_1, eqn\_a\_2, eqn\_b\_1, eqn\_b\_2, eqn\_c\_1, eqn\_c\_2$ we obtain the coefficients $F_l, l \geq 1$, needed for the evaluation of the potential Ux_d.

```
> coeff_x := solve({eqn_a_1,eqn_a_2,eqn_b_1,eqn_b_2,eqn_c_1,eqn_c_2},
> {A[l], B[l], C[l], D[l], E[l], F[l]}):
> F[l] := subs(coeff_x, F[l]):
```

Next, we evaluate the potential produced by the current dipole Q_x outside of the surface $\|\mathbf{r}\| = c$ numerically. To obtain a fast numerical routine the Maple code for the coefficients F_l in the series representation of Ux_d can be translated into optimized C or FORTRAN code. Moreover, the Maple packages MacroC [4] and Macrofort [5], available from the share library, allow an automatic generation of complete and ready-to-compile programs for the evaluation of the potential Ux_d (see Ref. [6] for an example). A convergence criterion for determining the required number of terms to achieve a prescribed accuracy is discussed in Ref. [7]. Here, we use the first 10 terms of the infinite series representation to get numerical values for plotting purposes.

```
> Ux[d] := 'sum(F[l]/r^(l+1) * 'a_P(l, 1, cos(theta))'*cos(phi), l=1..10)';
```

$$Ux_d := \sum_{l=1}^{10} \frac{F_l\,\text{'a\_P}(\,l, 1, \cos(\,\theta\,)\,)'\cos(\,\phi\,)}{r^{(\,l+1\,)}}$$

The expression for Ux_d depends on the parameters $rQ, r, a, b, c, \sigma_0, \sigma_1, \sigma_2, \sigma_3, \theta, \phi$, and Q_x. For the evaluation of this expression we need a procedure for calculating the associated Legendre polynomials.

```
> with(orthopoly, P):
> a_P := proc(n,m,x)
>        local q;
>            if m = 0 then P(n,q) else diff(P(n,q),q $ m) fi;
>            sqrt(1-q^2)^m*";
>            subs(q = x,")
>        end:
```

Next, we express the spherical angles θ and ϕ of the postion vector $\mathbf{r}$ in terms of the cartesian coordinates (x, y, z)

```
> theta := arccos(z/r); phi:= arctan(y, x);
```

$$\theta := \arccos\left(\frac{z}{r}\right)$$

$$\phi := \arctan(\,y, x\,)$$

and introduce a function for inserting special values of the parameters $r, a, b, c, \sigma_0, \sigma_1, \sigma_2, \sigma_3, Q_x$, and rQ.

```
> parameter := u -> subs(r=8.8e-2, a=8.1e-2, b=8.5e-2, c=8.8e-2,
> sigma[0]=0.33, sigma[1]=4.2e-3, sigma[2]=0.33, sigma[3]=0,
> Q[x]=10e-9, rQ=7.5e-2, u);
```

$$parameter := u \to \text{subs}\Big(r = .088, a = .081, b = .085, c = .088, \sigma_0 = .33,$$
$$\sigma_1 = .0042, \sigma_2 = .33, \sigma_3 = 0, Q_x = .10\,10^{-7}, rQ = .075, u\Big)$$

The physical units used are m (meter) for the length, Am (A Ampère) for the dipole moment, $(\Omega m)^{-1}$ (Ω Ohm) for the conductivities σ and V (Volt) for the potential. We select 10 nAm (n = nano = 10^{-9}) as dipole intensity, the order of magnitude usually required to explain the measured electric and magnetic field strengths outside of the head. In Figures 2 and 3 the contour lines of the electric potential $U_d = Ux_d$ on the top half of the sphere with radius $r = c$ are plotted in the x-y plane ($z = 0$).

```
> U[d] := subs(z=sqrt(r^2-x^2-y^2), parameter(Ux[d])):
> r := parameter(c);
```

$$r := .088$$

```
> plot3d(U[d], x=-r..r, y=-sqrt(r^2-x^2)..sqrt(r^2-x^2),
> labels=[x, y, V], style=contour, contours=[-3e-06+i*0.25e-6 $ i=0..24],
> colour=white, orientation=[-90,0], grid=[48,48], axes=frame);
```

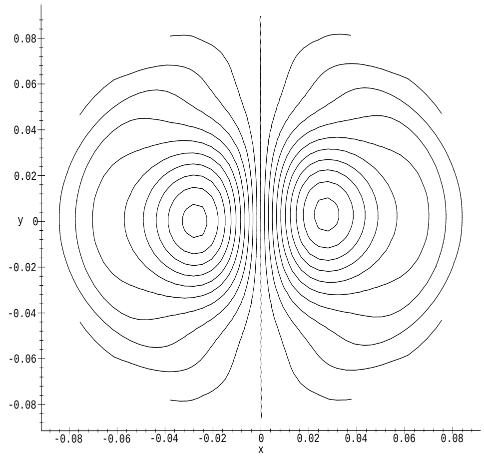

Figure 2: Dipole-envoked potential on the upper hemnisphere of the outermost surface of a three-layer spherical volume conductor model represented as contour map in the x-y plane. The step between successive isopotential lines is 0.25 μV (μ = micro = 10^{-6}).

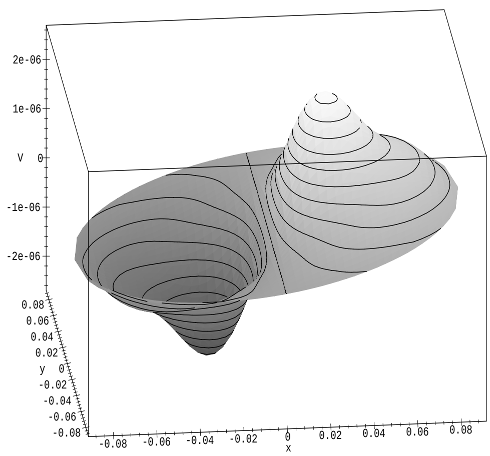

Figure 3: 3D contour map of the potential distribution shown in Fig. 2 (plot3d options used: **style=patchcontour, shading=zgreyscale**). The dipole Q_x near the skull layer generates a potential that peaks roughly along the axis of the dipole moment.

Conclusion

It has been shown how Maple can be used as a working environment for investigating mathematical models in the field of electroencephalography (EEG). EEG is a non-invasive method for estimating the location, orientation, and strength of current sources in the brain from measurements of the electric potential on the surface of the head (inverse problem). This estimation requires the solution of the forward problem, i.e., calculation of the electric potential due to known current sources in a specified conducting volume. At present, most EEG studies assume that the head is composed of spherical layers, each having a (different) constant value of electrical conductivity. In this article the EEG forward problem is solved analytically for a three-layer spherical model. Symbolic calculations are used for setting up the model equations, for the analytical solution of a sytem of linear equations, and for code generation to obtain a fast numerical program for the evaluation of the potential. Also, parametric studies using Maple's graphic capabilities are indicated. The applied computation technique is readily extended to the four-layer model or the general n-layer model. A worksheet version of this article will be available in the Maple share library.

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